

On the logarithmic oscillator as a thermostat

Marc Meléndez

*Dpto. Física Fundamental, Universidad Nacional de Educación a Distancia,
Madrid, Spain.*

Abstract

Campisi, Zhan, Talkner and Hänggi have recently proposed [1] the use of the logarithmic oscillator as an ideal Hamiltonian thermostat, both in simulations and actual experiments. However, the system exhibits several theoretical drawbacks which must be addressed if this thermostat is to be implemented effectively.

1 The logarithmic oscillator

A logarithmic oscillator is a point mass m in a central logarithmic potential. The Hamiltonian for such a particle is

$$H_{osc.}(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + k_B T \ln \left(\frac{\|\mathbf{q}\|}{b} \right) = E, \quad (1.1)$$

where $k_B T$ and b can be considered arbitrary parameters for the time being. The Hamiltonian equations of motion are therefore

$$\begin{cases} \dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m}, \\ \dot{p}_i = -\frac{\partial H}{\partial q_i} = -k_B T \frac{q_i}{q^2}. \end{cases} \quad (1.2)$$

This mechanical system has several interesting properties.

In the one-dimensional version of the oscillator, it is particularly easy to find the equations of motion by direct integration (we will disregard the singularity in the potential for the moment). From (1.1), we get the value of the momentum,

$$p = \sqrt{2m \left(E - k_B T \ln \left(\frac{q}{b} \right) \right)},$$

and using the first of Hamilton's equations of motion (1.2),

$$\dot{q} = \sqrt{\frac{2}{m} \left(E - k_B T \ln \left(\frac{q}{b} \right) \right)},$$

we get a differential equation which can be solved by separation of variables

$$t = \sqrt{\frac{m}{2}} \int \frac{dq}{\sqrt{E - k_B T \ln \left(\frac{q}{b} \right)}}. \quad (1.3)$$

Now, the amplitude of the oscillation is determined by the points q_α that satisfy the following equation:

$$k_B T \ln \left(\frac{q_\alpha}{b} \right) = E,$$

that is,

$$\begin{aligned} q_A &= -be^{\beta E}, \\ q_B &= be^{\beta E}, \end{aligned}$$

where β represents $(k_B T)^{-1}$. The period of oscillation is just twice the time taken by the particle to go from q_A to q_B ,

$$2t_{AB} = \sqrt{2m} \int_{q_A}^{q_B} \frac{dx}{\sqrt{E - k_B T \ln \left(\frac{|q|}{b} \right)}}. \quad (1.4)$$

The function in the integral is even, so

$$\begin{aligned} 2t_{AB} &= \sqrt{8m} \int_0^{q_B} \frac{dx}{\sqrt{E - k_B T \ln \left(\frac{q}{b} \right)}} \\ &= \sqrt{\frac{8\pi m}{k_B T}} be^{\beta E}. \end{aligned}$$

In the more general case, the motion of the particle lies on a plane. If it moves in circular orbits around the singularity with a radius r , then its velocity can be deduced from the fact that the central and centrifugal forces must balance,

$$F = \frac{k_B T}{r} = m \frac{v^2}{r}.$$

Therefore, the speed

$$v = \sqrt{\frac{k_B T}{m}} \quad (1.5)$$

does not depend on the radius of the orbit. The radius of the orbit is a function of the total energy E , because inserting (1.5) into (1.1), setting q equal to r and then solving for r gets us

$$r = \frac{be^{\beta E}}{\sqrt{e}}.$$

Therefore, the time it takes the particle to complete an orbit is

$$t_{orb.} = \frac{2\pi r}{v} = 2\pi \sqrt{\frac{m}{ek_B T}} be^{\beta E}.$$

For arbitrary initial conditions, the trajectory followed by the oscillator will not usually be a closed path, but the particle will never move further out than

$$r_{max.} = be^{\beta E},$$

for a given energy E , and the time between two consecutive maximum distances will be somewhere between $2t_{AB}$ and $t_{orb.}$ (note that both times are of the same order of magnitude),

$$\frac{2t_{AB}}{t_{orb.}} = \sqrt{\frac{2e}{\pi}}. \quad (1.6)$$

2 Statistical properties

The fact that the speed on a circular orbit does not depend on the radius is quite surprising. It implies that, if an external perturbation were to relocate the oscillator on a new circular orbit, the kinetic energy would remain the same and all the energy absorbed would be completely converted into potential energy.

In a sense, this result can be generalised to the oscillator's other trajectories. If we define the virial G as

$$G = pr, \quad (2.1)$$

and calculate its time derivative using (1.2),

$$\frac{dG}{dt} = p\dot{r} + \dot{p}r = 2 \left(\frac{p^2}{2m} \right) - k_B T.$$

The time average of the previous formula is

$$\left\langle \frac{dG}{dt} \right\rangle_t = 2 \left\langle \frac{p^2}{2m} \right\rangle_t - k_B T,$$

and if $\langle dG/dt \rangle_t = 0$, then the average kinetic energy must be

$$\left\langle \frac{p^2}{2m} \right\rangle_t = \frac{1}{2} k_B T, \quad (2.2)$$

whatever the value of E ! This means that the logarithmic oscillator can absorb an arbitrary amount of energy without changing its temperature at all, behaving (in a way) like an ideal thermostat.

Is it true, then, that $\langle dG/dt \rangle_t = 0$? It certainly is, as

$$\begin{aligned} \left\langle \frac{dG}{dt} \right\rangle_t &= \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \frac{dG}{d\tau} d\tau \\ &= \lim_{t \rightarrow \infty} \frac{G(t) - G(0)}{t} = 0, \end{aligned} \quad (2.3)$$

because G has upper and lower bounds, as one can see by noting that G is a continuous function, except at the origin. Given that

$$\begin{aligned} \lim_{r \rightarrow 0} G(r) &= 0, \\ G(r_{max.}) &= 0, \end{aligned}$$

we can infer that $G(r)$ has upper and lower bounds in the interval $(0, r_{max}]$, and (2.2) is correct. However, we must not forget that there is a limiting process involved in (2.3), and hence it might take a very long time for the average kinetic energy to converge to $k_B T/2$. In fact, we will argue that this is generally the case, and that the logarithmic oscillator is therefore a somewhat less-than-ideal thermostat.

A recent article in the arXiv [1] argued that weak coupling between a system of interest and a logarithmic oscillator will result in canonical sampling of the former's phase space. The dynamics of the compound system would then be determined by a total Hamiltonian

$$\begin{aligned} H(\mathbf{q}, \mathbf{p}, r, p_r) &= H_S(\mathbf{q}, \mathbf{p}) + H_{osc.}(r, p_r) \\ &\quad + H_{int.}(\mathbf{q}, \mathbf{p}, r, p_r) = E, \end{aligned}$$

where $H_S(\mathbf{q}, \mathbf{p})$ is the Hamiltonian for the system of interest, $H_{osc.}(r, p_r)$ is the one-dimensional version of (1.1), and $H_{int.}$ is the potential energy of the weak interaction between the system and the oscillator, which we will assume is negligible compared to H_S and $H_{osc.}$. The density of states for the logarithmic oscillator is

$$\Omega_{osc.}(E_{osc.}) = \int \delta(H_{osc.}(r, p_r) - E_{osc.}) dp_r dr,$$

with δ representing the Dirac delta function. The integral turns out to be exactly the same as (1.4), so

$$\Omega_{osc.}(E_{osc.}) = \sqrt{\frac{8\pi m}{k_B T}} be^{\beta E_{osc.}}. \quad (2.4)$$

Furthermore, the probability density ρ for a point in the phase space of the system corresponding to H_S is

$$\rho(\mathbf{q}, \mathbf{p}) = \frac{\Omega_{osc.}(E - H_S(\mathbf{q}, \mathbf{p}))}{\Omega(E)}. \quad (2.5)$$

The function $\Omega(E)$ represents the density of states of the compound system,

$$\Omega(E) = \int \delta(E - H(\mathbf{q}, \mathbf{p}, r, p_r)) dr dp_r d\mathbf{q} d\mathbf{p}. \quad (2.6)$$

Expressions (2.4) and (2.6) can be used to convert (2.5) into

$$\rho(\mathbf{q}, \mathbf{p}) = \frac{e^{-\beta H_S(\mathbf{q}, \mathbf{p})}}{\int e^{-\beta H_S(\mathbf{q}, \mathbf{p})} d\mathbf{q} d\mathbf{p}},$$

which is precisely the canonical distribution for H_S .

According to the authors of [1], the logarithmic oscillator thermostat has two obvious advantages. Firstly, contrary to the popular Nosé-Hoover thermostat, the dynamical equations of motion are Hamiltonian. Secondly, it is possible to design experimental setups in which the thermostat is an actual *physical* system. Hoover wrote a reply [2] to the first claim arguing that Nosé-Hoover mechanics *are* in fact Hamiltonian, and included an example of an alternative Hamiltonian thermostat of the Nosé-Hoover type. Campisi *et alii* answered explaining their claim further in [3]. Here we will be considering the second claim instead, that is, we will concentrate on the implementation of the logarithmic oscillator as a thermostat, both in experiments and simulations.

3 Experiments

An experimental thermostat that relies on the dynamics of only a few degrees of freedom is no doubt a very interesting system. However, the nature of the logarithmic oscillator imposes some serious limitations which must be taken into account before one attempts to design such an experiment.

The first problem is a consequence of the length-scales involved. Assume that we wish to bring a system with N degrees of freedom to the equilibrium temperature T . If the kinetic energy per degree of freedom is initially off by a fraction α of the energy,

$$\left\langle \frac{p_i^2}{2m} \right\rangle_t = (1 + \alpha) \frac{1}{2} k_B T,$$

then the logarithmic oscillator will have to absorb at least an amount of energy equal to $\Delta E = N\alpha k_B T/2$. We have seen that the oscillator typically covers distances of the order of $b \exp\{\beta E_{osc}\}$. The change in energy implies that the distances covered will change by

$$\Delta r_{max.} = r_{max.} (e^{\beta \Delta E} - 1). \quad (3.1)$$

This can be problematic if $r_{max.}$ is initially comparable to the size of the experimental apparatus and the oscillator is cooling the system.

The enormous changes in lengths imply similar changes in time scales. Having assumed a weak interaction between the system of interest and the oscillator, the effect of the interaction on the latter during one period of oscillation should not be significant. The period is

$$t_{per.} = \lambda \sqrt{\frac{m}{k_B T}} b e^{\beta E_{osc.}},$$

where λ is a factor that depends on the trajectory, but which is of the order of magnitude of $\sqrt{8\pi}$, in agreement with (1.6). The change in distances carries with it a corresponding change in periods of oscillation,

$$\Delta t_{per.} = t_{per.} (e^{\beta \Delta E} - 1). \quad (3.2)$$

Therefore, when the oscillator is cooling down the system of interest, it will usually move very far out and oscillate very slowly. On the other hand, when it is “hotter” than the system, it will squeeze into a small neighborhood of the singularity and vibrate very quickly.

Let us illustrate the problem with some numbers. The authors of [1] propose an experiment in which a small system composed of neutral atoms is contained in a box of length L . The logarithmic oscillator is an ion in a two-dimensional Coulomb field generated by a charged wire.

Assume, for example, that we have a dilute gas of 10 atoms of argon at an initial temperature $T_0 = 3$ K and that we wish to bring them to $T = 1$ K. This means that the logarithmic oscillator must absorb about

$$\Delta E = \frac{3}{2} N k_B T_0 - \frac{3}{2} N k_B T = 30 k_B T \quad (3.3)$$

units of energy. Let us assume further that the cross section of the charged wire has a radius equal to $10^{-3} L$. Then the logarithmic oscillator must move in orbits with

$$r_{max.} > 10^{-3} L.$$

However, when we insert (3.3) into (3.1) we find that

$$\Delta r_{max.} = r_{max.} (e^{30} - 1) > 10^{10} L.$$

If we also take equation (3.2) into account, it is easy to see that we should expect to find the oscillator outside the box most of the time.

4 Simulations

The wide range of time and length scales affects the precision and time of computation of numerical simulations as well, but the presence of a singularity in the logarithmic potential introduces another complication in the numerical implementation of the oscillator, as stepping over the singularity will usually lead to the wrong energy $E_{osc.}$.

When the particle is in the vicinity of the singularity, the slope $\partial H / \partial r$ changes very quickly. If the oscillator ends up too close to the singularity, it

will feel a great force which will push it away from the singularity during the next time step, making it skip the area in which the potential would slow it down again, unless a very small time step is chosen.

For the one-dimensional version of the logarithmic oscillator, the problem can be solved by calculating the new position of the logarithmic oscillator first. If the oscillator has stepped over the singularity, then expression (1.3) can be used to calculate the time it would have taken to get to the new position, and one can reset its kinetic energy to the correct value and calculate the evolution of the system of interest during that time. This solution is far from satisfactory, though, because it involves finding numerical values of the error function every time the particle passes the singularity.

A different approach ([1]) replaces the logarithmic potential with the approximate potential

$$V(r) = \frac{1}{2}k_B T \ln\left(\frac{r^2 + b^2}{b^2}\right),$$

thereby eliminating the singularity and introducing only a slight correction in the density of states for low values of $E_{osc.}$. Unfortunately, this imposes a limit on the amount of energy available for exchange between the oscillator and the system. If the system and oscillator are enclosed in a box of length L , one only has about $k_B T \ln(L/b)$ units of energy to play with. In order to allow for larger energy ranges, one must choose smaller values of b (of the order of $\exp\{-2\alpha 3N\}$ if we wish to allow the energy to fluctuate by a fraction α either way), and this will tend to generate a small neighbourhood of $r = 0$ in which the forces on the oscillator are huge.

5 Conclusions

The logarithmic oscillator proposed by Campisi, Zhan, Talkner and Hänggi displays very interesting

properties from the point of view of theoretical statistical mechanics. However, before it can be used as a thermostat in actual experiments and numerical simulations, three problems must be addressed. Firstly, the distances covered by the oscillator depend exponentially on its energy. Given that it must not interact strongly with container walls or other objects, one would expect that it would be very difficult to control such a system in practice. Secondly, the vast increase in the period of oscillation when a system is being cooled down suggests that the desired thermostated dynamics will be achieved very slowly. Lastly, the presence of a singularity introduces some technical complications in the numerical implementation of the dynamical behaviour of the oscillator. It seems, therefore, that Nosé-Hoover dynamics will remain a popular option in molecular dynamics at least until the problems mentioned here are resolved satisfactorily.

Acknowledgments

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References

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